Acetaldehyde
75-07-0 | DTXSID5039224

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.40

Global applicability domain: Inside

Local applicability domain index: 5.47e-01

Confidence level: 7.26e-01

Nearest Neighbors from the Training Set

Image not found
N,N-Dimethylformamide
Measured: 7.94e-01
Predicted: 1.12

Image not found
Diethyl ether
Measured: 5.37
Predicted: 4.72

Image not found
1,4-Dioxane
Measured: 5.01e-01
Predicted: 1.06

Image not found
Furan
Measured: 5.01
Predicted: 4.88

Image not found
2-Nitropropane
Measured: 8.32
Predicted: 7.41